ORDER AND CHAOS IN QUANTUM IRREGULAR SCATTERING: WIGNER'S TIME DELAY

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INTRODUCTION

Nearly thirty years of chaos research have shown that chaos is an ubiquitous phenomenon. Almost any dynamical system with a sufficiently large phase space described by nonlinear equations shows some kind of complexity in its time evolution, i.e. chaos. The degree of complexity is measured by topological entropy, Lyapunov exponents, decay of correlations, and, in the case of dissipative systems, various fractal dimensions. Examples abound, ranging from nonlinear oscillators to hydrodynamical systems and the motion of planets and asteroids (Schuster 1988). Nevertheless, these investigations have also revealed significant differences between an irregular looking chaotic signal and a really and truly random one, due to 'order within chaos' (the title of a conference, Campbell and Rose 1983, and a book, Bergé, Pomeau and Vidal 1988). One particular example of this order and coherence in chaos will be exploited below.

The fascination excerted by 'quantum chaos' and the controversy that surrounds it derives partly from the fact that according to the above measures, there is no chaos! For once, there is no nonlinearity in the Schrödinger equation. Secondly, quantal spectra of bounded systems are discrete, so that the time evolution of any observable is multiply periodic. On the other hand, the classical time evolution of chaotic systems is described by a non degenerate continuous spectrum, which is capable of rapid dephasing and decay (Cornfeld, Fomin and Sinai 1982). Since according to Ehrenfest's theorem, classical and quantum observables evolve alike for short times, one expects to see differences between classical and quantum behaviour after times T sufficiently long to resolve the discreteness of the quantum spectrum. [1] One now could try to develop measures that characterize the transient chaos-like properties of quantum systems whose classical counterpart shows chaos [2] or focus on generic properties of quantum systems in analogy to chaos being the generic property of classical systems (e.g. Eckhardt 1988a).

Alternatively, one may use the association 'chaos = irregularity' and ask whether one can identify within wave theory properties that give rise to irregularities of some kind. A hint is provided by wave optics: a superposition of a sufficient number of rays or waves leads to irregular speckle patterns. This analogy has been studied by O'Connor, Gehlen and Heller (1987), who also found a difference between patterns due to interference of waves with random amplitudes and

[1] This is an optimist's estimate. A pessimist might estimate the turnover time from the evolution of Gaussian wavepackets and conclude that it goes like $\log(1/\hbar)$ because of exponential spreading (Berry and Balazs 1979). Recent work by Tomsovic and Heller (1991) seems to support the optimist's version.

[2] Since there is no intrinsic definition, the correspondence to a classical system is required, with all its limitations and pecularities as for example in the case of spin systems (Graham and Höhnerbach 1984).

phases (as in the usual optical speckles) or due to waves with random phases but fixed amplitudes (the case relevant for quantum waves in billiards). This line of thought leads to random matrix theory (Haake 1991).

For quantum systems, the equivalent of light rays is provided by the semiclassical propagator, which expresses the transition amplitude from one point to another in a given time interval as a sum over all classically allowed paths connecting the two points in that time (Miller 1974). This semiclassical propagator in the time domain has attracted some attention recently (Tomsović and Heller 1991). In most cases, however, one transforms from the time domain to the energy domain and takes the trace which then allows one to study the spectrum of energy eigenvalues of the system (Gutzwiller 1967, 1969, 1970, 1971, 1990). In one degree of freedom one ends up with the WKB method (for phase shifts, propagators, quantization rules etc.), which is known to provide accurate and useful estimates (Berry and Mount 1972).

In many degree of freedom chaotic systems the semiclassical analysis leads to a relation between the quantum eigenvalues and classical periodic orbits (Gutzwiller 1990). The analysis is not easy to carry through to the end, with a quantization rule as simple as WKB as the final answer, since the number of periodic orbits grows exponentially with period, thus prohibiting a direct evaluation (Eckhardt and Aurell 1989). To some extend this exponential proliferation is the cause for irregular features in quantum systems, especially in the wavefunctions (Voros 1976, Berry 1977).

However, one also has a semiclassical expression, which in principle should be quantitatively useful when Planck's constant is sufficiently small, the de Broglie wavelength sufficiently short. The problem is how to tame the exponential proliferation of terms, that is, how to overcome the 'topological pressure' (Ruelle 1978, Gaspard 1992) or the 'entropy barrier' (Berry and Keating 1990). This problem occurs in a variety of contexts also outside semiclassical mechanics and techniques have been developed to overcome exactly this proliferation problem (Artuso, Aurell and Cvitanović 1990a,b). Below I will demonstrate both the taming of exponential proliferation of classical orbits and the emergence of irregular features for the time delay in scattering. I will do so for a specific model, scattering off three disks, that has proven extremely useful in developping and testing a number of concepts in chaotic scattering (Eckhardt 1987, Gaspard and Rice 1989a,b,c, Cvitanović and Eckhardt 1989, Eckhardt et al 1992, Eckhardt and Russberg 1992, Tanner et al 1991).

WIGNER'S TIME DELAY

The quantity for which I shall discuss the semiclassical expansion is Wigners time delay (Wigner 1955). As discussed by Wigner (single scattering channel) and Smith (1960) (many channels),it describes the phase difference between a scattered wave and a freely propagating one (though with the same asymptotic motion and thus with perhaps a single reflection in the interaction region, cf. Narnhofer and Thirring 1981). It controlls the absorption in a scattering experiment (Doron and Smilansky 1992, Doron, Smilansky and Frenkel 1991) and is of some relevance to persistent currents in mesoscopic rings (Akkermans et al 1991).

In terms of the S-matrix, the time delay $\tau(k)$ is given by

$$\tau = -i\hbar \, \mathrm{tr} \, S^\dagger \frac{\partial S}{\partial E} = -i\hbar \frac{\partial}{\partial E} \ln \det S \,. \tag{1}$$

The semiclassical expression is identical to Gutzwillers (1990) density of states (i.e. the excess density of states above a uniform background) and has been mentioned by Balian and Bloch (1974). For the billiard problem studied here, energy and Planck's constant only appear in the combination of the wavenumber, $k = \sqrt{2mE}/\hbar$ (m is the mass of the particle). When expressed in terms of wavenumber rather than energy, the time-delay becomes a 'length'-delay, viz.

$$\tau(k) = \tau_0(k) + \mathrm{Re} \, \sum_p \sum_{r=1}^{\infty} L_p \frac{e^{iL_p kr - i\mu_p \pi r/2}}{\sqrt{|\det(1 - M_p^r)|}} \,. \tag{2}$$

As usual in periodic orbit theory (Gutzwiller 1990, Eckhardt 1992), the semiclassical expression splits into a smooth part ($\tau_0(k)$) and a fluctuating part ($\tau_f(k)$) determined by periodic orbits. Since we have expressed everything in terms of wavenumber k rather than energy E, the time delay contains the geometrical length L_p of the trapped trajectory, the Maslov phase μ_p and the linearization perpendicular to the orbit M_p. The summation on r accounts for multiple traversals of an orbit. This expression is very similar to the classical trapping time distribution, where the amplitude of a trapped periodic orbit would be $1/|\det(1 - M_p^r)|$, i.e. without the square root and phases (Kadanoff and Tang 1984). This difference reflects the one between a quantum amplitude and a classical probability.

For the two degree of freedom systems considered below, M_p has eigenvalues Λ_p and $1/\Lambda_p$ (by convention, $|\Lambda_p| > 1$). Using an expansion of Miller (1975) for the determinant, one can express of the time delay as a logarithmic derivative of an infinite product:

$$\begin{aligned}
\tau_f(k) &= \mathrm{Re} \, \sum_p \sum_{r=1}^{\infty} \frac{-i}{r} \frac{\partial}{\partial k} \frac{e^{iL_p kr - i\mu_p \pi r/2}}{\sqrt{|\det(1 - M_p^r)|}} & (3) \\
&= \mathrm{Re} \, i \frac{\partial}{\partial k} \sum_p \sum_{j=0}^{\infty} \sum_{r=1}^{\infty} \left(-\frac{1}{r}\right) \left(e^{iL_p k - i\mu_p \pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}\right)^r & (4) \\
&= \mathrm{Re} \, i \frac{\partial}{\partial k} \sum_p \sum_{j=0}^{\infty} \log\left(1 - e^{iL_p k - i\mu_p \pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}\right) & (5) \\
&= \mathrm{Re} \, i \frac{Z'(k)}{Z(k)} & (6)
\end{aligned}$$

where the prime denotes a derivative with respect to wavenumber k and

$$Z(k) = \prod_p \prod_{j=0}^{\infty} \left(1 - e^{iL_p k - i\nu_p \pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j}\right) \tag{7}$$

Fig. 1: Proliferation of periodic orbits with period for the three disk system for different distance to radius separations. From top to bottom: $d : R = 2.5$, 2.8, 3, 4, 5 and 6.

is a Selberg type zeta function (Selberg 1956, Voros 1988), named after similar expressions in the theory of motion on surfaces of constant negative curvature (Balazs and Voros 1986).

The technical difficulty with this expression is the exponential proliferation of periodic orbits, as mentioned before. For the three disk billiard, this is easily seen from the topology of trajectories: After leaving a disk, the particle has two choices for the next collision. Thus the number of orbits grows like $3 \cdot 2^{n-1}$ with n the number of collisions (there are three choices for the first and two for the following ones) (Eckhardt 1987, 1992). Taking into account an average length of paths between collisions, this translates into an exponential proliferation with length (Fig. 1).

For practical calculations it is now useful to group terms according to their topological length. Technically, one introduces a counting variable z^{n_p} where n_p is the topological period of the orbit and expands

$$Z(k) = \sum_p \sum_{r=1}^{\infty} L_p \frac{e^{iL_p kr - i\nu_p \pi r/2}}{\sqrt{|\det(1 - M_p^r)|}} z^{n_p r} = \sum_n C_n(k) z^n \tag{8}$$

in a power series using formulas of Plemelj (1909) and Smithies (1941) (see also Reed and Simon 1983). In Figure 2 the coefficients $C_n(k)$ for various distance to radius ratios within the A_1 symmetry are shown. One clearly notes the rapid decay of coefficients with increasing n.

As a careful analysis of the coefficients $C_n(k)$ in (8) shows, all but the first few are combinations of long orbits with short orbits approximating the long ones (Cvitanović and Eckhardt 1989,

Fig. 2: Scaling of the coefficients in the cycle expanded Selberg zeta product (8). Shown is $\log_{10}|C_n(k=0)|$ vs. n for the same distance to radius ratios as in Figure 1.

Artuso, Aurell and Cvitanović 1989a,b, Eckhardt 1992, Eckhardt and Russberg 1992). If the index $a^n b$ describes the long orbit composed of n repetitions of a shorter one a and a second orbit b, then the expansion (8) will contain contributions of the form (e.g. for $j=0$)

$$e^{iL_{a^nb}k-i\mu_{a^nb}\pi/2}|\Lambda_{a^nb}|^{-1/2}\left(1-e^{i(L_{a^{n-1}b}+L_a-L_{a^nb})k}e^{-i(\mu_{a^{n-1}b}+\mu_a-\mu_{ab})\pi/2}\left|\frac{\Lambda_{a^nb}}{\Lambda_{a^{n-1}b}\Lambda_a}\right|^{1/2}\right) \tag{9}$$

The second term in the parenthesis contains only terms comparing the long orbit with the two approximants. In hyperbolic systems, orbits are by definition exponentially unstable. Thus to stay near an orbit for n traversals requires one to be exponentially close to it. Thus the difference between orbits $a^n b$ and $a^{n-1}b$ is one more traversal very (exponentially) close to a. Thus the differences in action are exponentially close to zero, the ratios in instabilities close to 1. If now the Maslov phases (a discrete quantity) fit as well (one can assure this by a proper choice of symbolic organization of orbits, Eckhardt and Wintgen 1991, Eckhardt 1992), all that enters in (9) are the deviations from one, i.e. an exponentially small quantity. This is enough to turn the expanded product (8) convergent for real energies.

This is a first example of order among all this chaos: long periodic orbits are not random numbers but are strictly correlated with shorter orbits, so that one can actually estimate the contributions from long orbits rather accurately and obtain convergent results for the density of states and related quantities.

For large n the decay is only exponential rather than superexponential, in contrast to the classical Selberg zeta function (Cvitanović and Eckhardt 1991). Techniques have been developed to improve this further to recover faster than exponential convergence (Eckhardt and Russberg

1992). A new semiclassical Selberg type product, similar to the classical one, is currently under investigation. Preliminary test indicate improved convergence. The calculations shown here were performed with the expansion (8) directly, using orbits of period up to 13.

One test of the semiclassical expression is to compare zeros of (8) with poles of the S-matrix. The result (Cvitanović and Eckhardt 1989, Eckhardt et al 1992) is that the differences between exact and semiclassical resonances decrease with increasing wavenumber, i.e. when approaching the semiclassical limit. This is in spirit with the semiclassical approximation and confirms that Gutzwillers (1990) analysis is a bona fide semiclassical theory.

A plot of the time delay for a larger interval in k shows large fluctuations, and lots of irregular features (Fig. 3). They come about because every resonance of the S-matrix contributes a Lorentzian to the time delay. If the positions of the resonances are $k_i = s_i - i\gamma_i$, then

$$\tau(k) = \sum_i \frac{\gamma_i}{(k - s_i)^2 + \gamma_i^2} \,. \tag{10}$$

Cross sections differ from the above expression in that the weights of the Lorentzians are not unity (Ericson 1960, Brink and Stephen 1963) and also show fluctuations. Signals of this kind were extensively studied in nuclear physics (Ericson 1960, Brink and Stephen 1963) in connection with the compound nucleus. It was shown that a correlation function contains information on the average widths of resonances and thus on the lifetime of the compound nucleus. A semiclassical interpretation has been attempted by Blümel and Smilansky (1988), starting directly from the S-matrix. In this limit, however, the same information should also be contained in the time delay and its correlation function (for a discussion of deviations in extreme quantum cases, see Lewenkopf and Weidenmüller 1991).

CORRELATION FUNCTIONS

Consider the fluctuating part of the time delay (after subtracting the mean), more precisely a segment $\tau_s(k) = \tau_f(k)w(k)$, projected out with a window function $w(k)$ (e.g. a box of width Δk centered around k_0 or a Lorentzian). The autocorrelation function of this segment is then given by the integral

$$C(\kappa) = \int_{\Delta k} dk\; \tau_s(k - \kappa/2)\, \tau_s(k + \kappa/2)\ . \tag{11}$$

Its Fourier transform $K(\lambda)$ is the structure function,

$$K(\lambda) = \int d\kappa\; C(\kappa)\;\; \cos(\kappa\lambda)\,. \tag{12}$$

Fig. 3: Time delay for scattering off the three disk system at $d : R = 2.5$. The lower frame shows a magnification and comparison between different maximal periods of orbits included.

Fig. 4: Autocorrelation function of the time delay for $d : R = 2.5$. It was computed for intervals of $\Delta\kappa = 50$ starting at the k-values indicated in the figure. For comparison, the bold line shows a Lorentzian of width $\gamma = 0.15$ (Eq. 14).

Since the time delay is a superposition of Lorentzians, the correlation function for small κ probes their widths. In a simplified analysis, assume that the window $w(k)$ selects a finite number of resonances in each $\tau(k)$. Then

$$C(\kappa) = \sum_i \sum_j \int dk \; \frac{\gamma_i}{(k - \kappa/2 - s_i)^2 + \gamma_i^2} \; \frac{\gamma_j}{(k + \kappa/2 - s_j)^2 + \gamma_j^2} \tag{13}$$

which, in the diagonal approximation, becomes

$$C(\kappa) = \sum_i \frac{2\gamma_i}{(\kappa - s_i)^2 + 4\gamma_i^2} \approx \frac{2\gamma}{\kappa^2 + 4\gamma^2} \,. \tag{14}$$

The last form is an approximation by a single Lorentzian of effective width 2γ.

Comparison with the computed autocorrelation function (Figure 4) shows that a Lorentzian describes the correlation function only for very small k. For larger ones, $C(\kappa)$ even becomes negative. A similar discrepancy was noted by Wardlaw and Jaworski (1989) in their analysis of the phase shift for a particle scattered off a leaky surface of constant negative curvature (a model introduced by Gutzwiller 1983). In a later study, Shushin and Wardlaw (1992) could actually improve on the form of $C(\kappa)$ by adding correlations between the positions of resonances, predicting a correlation function of the form

$$C_{SW}(\kappa) \approx \gamma^2 \frac{\gamma^2 - \kappa^2}{(\kappa^2 + \gamma^2)^2} \,. \tag{15}$$

Fig. 5: Structure function for the time delay shown in Figure 3. The inset shows the structure function over a larger range on a logarithmic scale. Clearly visible is the exponential fall off related to the Lorentzian of the autocorrelation function.

This form does not fit the data any better, presumably because the underlying ensemble of resonances is different from the assumed GUE ensemble (see e.g. Haake 1991).

The large κ behaviour of the correlation function is difficult to access from the resonance representation (10). This behaviour on the other hand is reflected in the small λ behaviour of the structure function. Using the semiclassical representation (2) for the time delay, the structure function for a segment $\tau_s(k)$ becomes

$$K(\lambda) = \left| \sum_p \sum_{r=1}^{\infty} \frac{L_p e^{-i\nu_p \pi r/2}}{\sqrt{|\det(1 - M_p^r)|}} \tilde{w}(\lambda - rL_p) \right|^2 \tag{16}$$

$$= \sum_p \sum_{r=1}^{\infty} \frac{L_p^2}{|\det(1 - M_p^r)|} \tilde{w}^2(\lambda - rL_p) + \sum_P \sum_{P'} A_P A_{P'}^* \tilde{w}(\lambda - L_P) \tilde{w}(\lambda - L_p)\,, \tag{17}$$

where $\tilde{w}$ is the Fourier transform of the window function; P and P' denote periodic orbits (perhaps multiple traversals of shorter ones) with weights A_P, $A_{P'}$ and of length L_P and $L_{P'}$, respectively. If the window is sufficiently wide, then the Fourier transform will be narrow and no terms will overlap when taking the absolute value squared. Therefore, only the diagonal contributions in (17) survive and the structure function will show individual periodic orbits for small λ. For very large λ, interferences between different periodic orbits will eventually turn the sum into the exponential decay required by the Lorentzian result for the small τ behaviour of the correlation function.

RELATION TO BOUNDED SYSTEM

As the disks are moved close enough to touch, they enclose a region of the shape of a tipped triangle. Since this is a bounded system, it has a discrete spectrum. The Wigner time delay then turns into the density of states of the bounded system and the resonances become infinitely sharp. Semiclassical quantization attempts for this system have been reported elsewhere (Tanner et al 1991). Here I would like to describe the relation between the correlation function and structure function for the time delay as found above to the semiclassical theory of two point correlation functions by Berry (1985).

The small λ behaviour of the structure function with the periodic orbits is in agreement with Berry's semiclassical analysis and numerical results (e.g. Wintgen 1987). The large λ exponential decay is consistent with it, since the decay rate is related to the width of the resonances; in a bounded system, the widths goes to zero and $K(\lambda)$ settles to a constant (Levandier et al 1986, Pique et al 1987). What seems to be missing is the intermediate regime, where in a bounded system $K(\lambda)$ should increase linearly.

For λ large enough so that the periodic orbits overlap, but not too large so that the cancellations take over, the correlation function near λ sums over all orbits with length near λ,

$$K(\lambda) \approx \sum_{L_p \text{ near } \lambda} \frac{L_p^2}{|\det(1 - M_p^r)|} \approx \lambda e^{-\Gamma\lambda} \,. \tag{18}$$

The approximate form is valid for intermediate λ and contains the classical escape rate Γ (Kadanoff and Tang, 1984, Cvitanović and Eckhardt 1991), up to a factor L. In the case of bounded systems, $\Gamma = 0$ and $K(\lambda)$ increases linearly with λ. For open systems, it attains a maximum near $\lambda = 1/\Gamma$. For the three disk system at $d : R = 2.5 : 1$, $\Gamma \approx 0.7$, so that it is impossible to detect the intermediate classical region. However, the exponent Γ clearly does not describe the exponential decay for large λ, as speculated by Blümel and Smilansky (1988). Incidently, notice that in this case the quantum decay is *slower* than the classical decay. Thus the interferences between off-diagonal terms in (17) act to increase $C(\lambda)$ compared to the classical value and not to decrease it as in the case of the bounded system (Berry 1985).

CONCLUSIONS

Investigations in 'quantum chaos' and in particular on Gutzwiller's periodic orbit formula for the density of states have helped to uncover a considerable amount of order among irregular looking quantum data. The main tool is the Fourier transform which facilitates the transition from the energy domain to the time domain, where the dynamics is dominated by correlations; they give rise to longer range correlations in energy. I have demonstrated these ideas using as an example a simple scattering system, where one has good control over both classical and quantum dynamics and where it is possible to sum the semiclassical expressions, despite the exponential proliferation of orbits. The results confirm that the cycle expansion of Selberg products (8) provides a convenient and accurate method for the calculation of periodic orbit sums in hyperbolic systems. It has allowed for a accurate test of Gutzwiller' semiclassical theory.

A number of problems still remain. Among them are the extension of periodic orbit summation techniques to non-hyperbolic cases, the summation of expressions for cross sections and the extension to more degrees of freedom than just two (perhaps even field theories). I am optimistic that eventually, a semiclassical theory for chaotic systems, perhaps as useful and reliable as the well-known WKB methods, will emerge.

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